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The Lanczos Method Applied to Statistical Stark Broadening of Spectral Lines

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Abstract

The quasi-static ion approximation of Stark broadened spectral lines involves an average of the field-dependent line shape over the microfield probability distribution. In the conventional approach, this can become computationally expensive since the calculation at each field point requires inverting a possibly large matrix. It is shown that these calculations are well suited to the “Padé Via Lanczos” approach. The approach allows for an efficient and accurate numerical integration over the quasi-static field. In turn, the integration forms the basis for determining convergence with Lanczos iterations. Simple examples are used to demonstrate improved performance over conventional methods and note the potential for larger gains on more complex problems.

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1. Introduction

Computer codes have been developed to calculate Stark broadened line shapes from multi-electron ions extending the capabilities beyond one- or two-electron systems [1-4]. For large numbers of atomic levels these calculations can be computationally challenging. Although approximations to the physics have been introduced to mitigate the problem, [3] accurate results are necessary not only to validate approximate schemes, but also for cases not satisfying the approximation criteria.

Multi-electron ion codes usually make the quasi-static ion approximation where the ion motion is assumed negligible during the average lifetime of the radiating states [1-4]. Thus, the line shape calculation involves averaging the Stark state mixing and level splitting over the field distribution. In the absence of external fields the line shape can be written in the form [1-4],

$$I(\omega) = \int_0^{\infty} d\varepsilon P(\varepsilon) J(\omega; \varepsilon) \quad (1.1)$$

where $\hbar\omega$ is the energy of the photon, $P(\varepsilon)$ is the probability of finding a Stark field of magnitude ε at the radiator, and $J(\omega; \varepsilon)$ represents the line shape due to electron-radiator interactions in the presence of this field.

The numerical evaluation of the line shape replaces the integral in Eq. (1.1) with the sum

$$I(\omega) = \sum_{i=1}^{N_\varepsilon} w_i P(\varepsilon_i) J(\omega; \varepsilon_i) \quad (1.2)$$

where N_ε is the number of field points and w_i are weights appropriate to the integration scheme. In calculating Eq. (1.2) it is desirable to select a procedure that simultaneously yields sufficient accuracy and minimizes the computational effort. Recently a method [5] based on a Hessenberg decomposition was presented that is formally exact, numerically stable, and allows for the optimization of the field mesh.

The purpose here is to take advantage of that formulation, but instead apply the Lanczos process to evaluate $J(\omega; \varepsilon)$. The proposed method is similar to that used in large-scale linear systems involving non-Hermitian matrices [6] providing numerical stability with high efficiency compared to traditional calculations. It is stressed that the Lanczos process does not make any physical approximations; instead it is a reduced-order model containing a relatively small number of dominant eigenvalues. Numerical accuracy is controlled using a straightforward scheme to determine convergence of the Lanczos iterations. The procedure is sufficiently

efficient that an adaptive quadrature scheme for evaluating Eq. (1.1) may prove satisfactory. Alternatively, the Lanczos method can also reveal the structure of $J(\omega;\varepsilon)$ through a dispersion formula allowing optimization of the field mesh to perform accurately the numerical integration over Stark fields.

2. Padé Via Lanczos

The field-dependent line shape in Eq. (1.1) can be written in the form [5]

$$J(\omega;\varepsilon) = -\pi^{-1} \text{Im} \left\{ \ell^t [A(\omega) - \varepsilon B]^{-1} u \right\} \quad (2.1)$$

where ℓ and u are vectors simply related to the radiator dipole operator, t superscript denotes transpose, $A(\omega)$ represent line broadening in the absence of the quasi-static Stark field, and B depends only on the internal coordinates of the radiator. The form of Eq. (2.1) is amenable to the ‘‘Padé Via Lanczos’’ (PVL) method, which is an efficient, numerically stable algorithm [6].

2.1 Method

To proceed, rewrite Eq. (2.1) in the form

$$J(\omega;\varepsilon) = -\pi^{-1} \text{Im} \left\{ \ell^t [I - (\varepsilon - \varepsilon_o)C]^{-1} r \right\} \quad (2.1.1)$$

where I is the identity matrix,

$$r = [A - \varepsilon_o B]^{-1} u, \quad (2.1.2)$$

$$C = [A - \varepsilon_o B]^{-1} B, \quad (2.1.3)$$

ε_o is a reference expansion point, and the frequency dependence was suppressed for brevity.

The tridiagonal decomposition of the matrix C is accomplished by the Lanczos method [7], leading to

$$J(\omega;\varepsilon) = -\pi^{-1} \text{Im} \left\{ \ell^t Q [I - (\varepsilon - \varepsilon_o)T]^{-1} P^h r \right\} \quad (2.1.4)$$

with

$$C = QTP^h \quad (2.1.5)$$

$$QP^h = P^h Q = I \quad (2.1.6)$$

where h superscript denotes Hermitian conjugate and T is a tridiagonal matrix. All field independent quantities are evaluated once at each frequency. Then the calculation of $J(\omega;\varepsilon)$ at the required N_ε mesh points only requires the tridiagonal solve in Eq. (2.1.4).

Although Eq. (2.1.4) appears similar to the results using the Hessenberg decomposition [5], there are fundamental differences. By exploiting the remarkable properties of the Lanczos method, the PVL approach yields significant savings for large problems [6]. Ultimately, Eq. (2.1.4) can be written in the form [6,7]

$$J(\omega;\varepsilon) \approx J_k(\omega;\varepsilon) = -\pi^{-1} \text{Im} \left\{ \left(\ell^t r \right) e_1^t \left[I - (\varepsilon - \varepsilon_o) T_k \right]^{-1} e_1 \right\} \quad (2.1.7)$$

where $e_1 = [1, 0, \dots, 0]^t$ is the first unit vector of length k , the number of Lanczos iterations. This is an important result since only the [1,1] element of $[I - (\varepsilon - \varepsilon_o) T_k]^{-1}$ is required. Since T_k is a tridiagonal matrix, it is possible to derive a Padé expansion for the [1,1] element in terms of ε (hence, Padé Via Lanczos). In practice, however, the evaluation of Eq. (2.1.7) can be done with a recursion relation. Further details are provided in the Appendix.

2.2 Order-reduction and convergence

The Lanczos approach provides an approximation to $J(\omega;\varepsilon)$ that improves with the number of iterations until it reaches its best value when the number of iterations is equal to the size of the matrix C . A smooth function, however, can be satisfactorily reproduced with relatively few iterations. Thus, the smoothness of the function rather than the size of the matrix C determines the number of iterations. This order-reduction provides a significant computational advantage over traditional methods for large matrices and smooth functions.

Unfortunately, it is not possible to determine the optimal number of Lanczos iterations in advance. It is then necessary to use an incremental approach and continue iterating until a convergence criterion is satisfied. Here, a straightforward, physically motivated approach is used to determine convergence.

Start with a chosen number of iterations and perform the numerical integration in Eq. (1.2). Next increase the iterations by some increment and repeat the numerical integration procedure with the larger tridiagonal matrix. If the difference between this answer and the previous one is greater than a chosen tolerance, continue the iteration until the criteria is satisfied. The use of the integral as the convergence criterion is consistent with the overall goal, the evaluation of the line shape in Eq. (1.1).

In the above approach, there is no expense in the Lanczos procedure itself when increasing the number of iterations, since all the information can be stored and the process can be restarted without cost. One additional expense is the evaluation of the integral itself, however, this is a

small increase in operation count since the evaluation of $J(\omega;\varepsilon)$ is of order k . Thus, this convergence scheme is inexpensive and can be used at fairly small intervals in the Lanczos iterative scheme without adding significantly to the overall operation count.

It is stressed that the convergence procedure has not been demonstrated to be robust. Since it is possible that the procedure as described can display spurious convergence, it may be desirable to use more than two Lanczos iterations in the procedure. It should also be pointed out that the convergence behavior could be highly erratic, similar to that of iterative techniques such as bi-conjugate gradients for non-symmetric systems.

2.3 Orthogonality of Lanczos vectors

The discussion above highlights the attractive features of the Lanczos method for the evaluation of $J(\omega;\varepsilon)$. In finite precision arithmetic, however, the Lanczos method can rapidly lose the bi-Hermitian property of the Lanczos vectors and become unstable. To remedy the situation several schemes have been developed [7-9]. For simplicity, the readily implemented and robust Modified Gram Schmidt procedure is applied at each iteration (the equivalent of full orthogonalization for complex non-symmetric matrices [7]). Although in most Lanczos implementations full orthogonalization is rejected as too expensive, it is shown in Sect. 3.5 that full orthogonalization adds relatively little to the overall expense in the present application; hence, it is an excellent approach given the ease of implementation.

2.4 Efficient Stark field integration

An additional step is necessary in completing the algorithm. That is, the goal is not merely to evaluate $J(\omega;\varepsilon)$, but to average it over the microfield distribution. Since the evaluation of $J_k(\omega;\varepsilon)$ is inexpensive, one approach is to use an adaptive quadrature procedure to compute Eq. (1.1). Alternatively, it is possible to determine the location and widths of the peaks in the range of integration in advance. As described in [5], this is facilitated by knowing the eigenvalues of the matrix C , which are well approximated by those of the tridiagonal matrix T_k . In turn, the eigenvalues provide the poles of $J_k(\omega;\varepsilon)$ that can be used to optimize the field mesh in Eq. (1.2) [5].

2.5 Operation counts

It is useful to have an indication of the operation counts to determine the relative costs of the algorithm. Even though the matrices A and B are typically sparse, it is expedient to take an

operation count that ignores the sparsity; thus, leading to conservative estimates. In the following, all operation counts assume operations performed with complex numbers.

In each Lanczos iteration, the quantities

$$(A - \varepsilon_o B)^{-1} B \ell \quad (2.5.1)$$

and

$$\left[(A - \varepsilon_o B)^{-1} B \right]^h r \quad (2.5.2)$$

need to be evaluated. This is best achieved by an LDL^h factorization of the matrix $A - \varepsilon_o B$ [9]. Since $A - \varepsilon_o B$ is a symmetric matrix of rank m , the factorization operational count is $\sim m^3/3$ (neglecting lower order terms in m). In addition, there are $4m^2$ operations for the Lanczos vectors per iteration plus $2mk^2$ operations for k iterations to ensure the bi-hermitian property of the Lanczos vectors. Typically, the latter is an unacceptable expense and is almost invariably avoided. In the present situation, however, it is negligible compared to the LDL^h factorization cost as long as $k \ll m$. Thus, the total cost for performing k Lanczos iterations is approximately

$$N_k \approx \frac{m^3}{3} + 4m^2k + 2mk^2 \quad (2.5.3)$$

In the limit that the process is carried out to $k = m$ Lanczos iterations,

$$N_{k=m} \approx 6m^3 \quad (2.5.3)$$

This can be compared with $\sim 12m^3$ operations for the Hessenberg decomposition of the matrix C [5]. Furthermore, the calculation at each field point using the Hessenberg approach requires m^2 operations where solving Eq. (2.1.7) requires only $3k$ operations. Clearly, the approach using the Lanczos method is more efficient.

It is also worthwhile to compare the operation count to the conventional approach using explicit matrix version. In that case the operation count to perform the numerical integration is

$$N_I \approx N_\varepsilon m^3 \quad (2.5.4)$$

Adding to Eq. (2.5.3) the cost for solving the tridiagonal system gives for the total operation count of the PVL gives

$$N_L \approx N_k + 3N_\varepsilon k \quad (2.5.5)$$

Comparing to the conventional method yields the ratio

$$\frac{N_I}{N_L} \approx \frac{3N_\varepsilon}{1 + 12\frac{k}{m} + 6\frac{k^2}{m^2} + 9\frac{N_\varepsilon k}{m^3}} \xrightarrow{m \gg k, N_\varepsilon} 3N_\varepsilon \quad (2.5.6)$$

so that for large matrices and relatively smooth $J_k(\omega; \varepsilon)$ there is considerable savings. In the limit $k = m$

$$\frac{N_I}{N_L} \xrightarrow{k=m \gg N_\varepsilon} \frac{3N_\varepsilon}{19} \quad (2.5.7)$$

Even in the extreme iteration limit the PVL method is more efficient than the conventional approach.

It is interesting to note that for $k \ll m$ the main cost of the Lanczos method is in the LU factorization of the matrix $A - \varepsilon_o B$. In many situations, however, the interference terms are neglected making A a diagonal matrix [1-4]. Then it is possible by choosing $\varepsilon_o = 0$ to avoid the costly LU factorization. The penalty is a possible increase in the number of Lanczos operations to achieve convergence (see Sect. 3).

A cautionary remark is that the operation counts alone are not sufficient to determine the relative time for execution. That is, BLAS3 operations are often an order of magnitude faster than operations that have not been optimized and it is necessary to compare actual implementations to determine savings in execution time.

2.6 Calculations on a frequency mesh

The operation count analysis showed that for a relative small number of Lanczos iterations the most expensive aspect of applying the Lanczos process to statistical Stark broadening is the LDL^h factorization of the reference resolvent to solve equations of the form

$$(A - \varepsilon_o B)x = b \quad (2.6.1)$$

As an alternative, an iterative solver for sparse matrices may provide significant faster results [10]. In particular, the iterative solver is efficient if used with a suitable pre-conditioner. In spectral line broadening calculations the profile is computed on a frequency mesh; thus, a previous factorization at a nearby frequency point may provide a good pre-conditioner. The pre-conditioner may be useful for nearby frequency points until eventually the number of iterations may increase beyond an acceptable value. In that case, a new LDL^h factorization is performed and the process repeated.

Another way to take advantage of the frequency mesh is when choosing the reference field ε_o . That is, the expression obtained in the Lanczos process attempts to mimic the behavior of the exact Taylor expansion for Eq. (2.1.1) around the point $\varepsilon = \varepsilon_o$. Depending on the structure of the integrand in Eq. (1.1), it may be advantageous to expand around different values [6]. In general, the algorithm converges to the same result independent of the reference point, but the rate of convergence may depend on the choice of ε_o (see Sect. 3). Although it is not possible to know the ideal reference point beforehand, it should be adequate to use the solution from a previous value from a nearby ω as a suitable estimate.

3. Numerical example

The Balmer line series in hydrogen, which involves radiative transitions from principal quantum number $n \geq 3$ to $n = 2$, serves as simple example to illustrate the PVL approach. In the present calculation, off-diagonal terms of $\Phi(\omega)$ as well as line shifts from plasma electrons are neglected. The diagonal terms of $\Phi(\omega)$ are obtained using a standard approximation [11], where the strong collision parameter was extended to higher principal quantum numbers by assuming $C_n = 3/n$ for $n \geq 6$. The calculation of the matrix B in Eq. (2.1) neglects interactions between the upper and lower state manifolds of the radiative transitions; that is, includes all interactions except the terms connecting $n = 2$ and $n \geq 3$. The line series is calculated through $n = 20$ and the required radial dipole matrix elements are computed using recursion relations [12]. The integration in Eq. (1.1) assumed the Holtsmark distribution in the range $0 < \varepsilon \leq 25\varepsilon_H$ where ε_H is the Holtsmark field [13]. Since the evaluation of $J(\omega; \varepsilon)$ using the Lanczos process is relatively fast, the integration was performed with an adaptive quadrature (see Sect. 2.4). Finally, the discussion emphasizes a diagonal block with magnetic quantum number $m_\ell = 0$ of size $m = 414$.

Results for $J_k(\omega; \varepsilon)$ at $\hbar\omega = 3.02 eV$ for k Lanczos iterations using reference points $\varepsilon_o = 0$ and $2.4\varepsilon_H$ are displayed in Figs. 1 and 2, respectively. The frequency corresponds to a spectral location in the red wing of the H_δ ($n = 6$) line. The calculations are done for free electron density $N_e = 10^{16} cm^{-3}$ and temperature $T = 1 eV$ so that the H_δ line is below the Inglis-Teller limit [14], but there is still significant Stark mixing between states of different principal quantum number. The two figures show the sensitivity of the results to the reference point. The choice $\varepsilon_o = 2.4\varepsilon_H$, which is at the first maximum in $J(\omega; \varepsilon)$ and occurs not far from the peak of the Holtsmark distribution function, displays a faster rate of convergence with increasing k . This

is confirmed in Fig. 3 where the integration of Eq. (1.1) as a function of Lanczos iterations is compared to the exact result (here exact denotes calculations using the conventional method). Note that even the $k = 5$ Lanczos results only produce $\sim 1.5\%$ error. The explanation follows from Fig. 4 where the integrand of Eq. (1.1) is plotted showing that the variations in $J_k(\omega; \varepsilon)$ for different k occur in the tail of the microfield distribution and have a small effect on the integration. The results suggest that high accuracy can be achieved with $k \approx 35$, that is a considerable order-reduction compared to the original size of the matrix, $m = 414$.

Similar calculations are presented in Figs. 5 through 8 for $\hbar\omega = 3.05 eV$ located in the blue wing of the H_δ line. Figures 5 and 6 show that the first peak in $J(\omega; \varepsilon)$ is further away from the peak of the distribution, $\varepsilon \approx 7\varepsilon_H$. These two figures display calculations using $\varepsilon_o = 0$ and $7\varepsilon_H$ and again show sensitivity to the reference point. The convergence of the integration in Eq. (1.1) is displayed in Fig. 7, which as suggested by Figs. 5 and 6, shows that the choice $\varepsilon_o = 7\varepsilon_H$ has a faster rate of convergence. The integrand of Eq. (1.1) at $\hbar\omega = 3.05 eV$ is displayed in Fig. 8 showing that the variations in $J_k(\omega; \varepsilon)$ occur in the tail of the microfield distribution not significantly affecting the error in the integration; hence, even for $k = 5$ the error is less than 7%. As in the previous case, accurate results can be obtained with $k \approx 35$ Lanczos iterations.

It is stressed that the convergence in Figs. 3 and 7 is not monotonic with increasing number of Lanczos iterations. Consequently, a robust convergence criterion will have to account for this possibility. These results also show sensitivity to the reference point, ε_o . Although a systematic choice was not determined, results selecting the value of ε_o near the peak of $J(\omega; \varepsilon)$ produce faster convergence than simply choosing $\varepsilon_o = 0$. Note, however, that the results for $J_k(\omega; \varepsilon)$ using $\varepsilon_o = 7\varepsilon_H$ are starting to show discrepancies near $\varepsilon = 0$ for $k = 5$. This emphasizes that the Lanczos process is expanding about the reference point and probably should not be chosen far from the peak of the microfield distribution.

4. Conclusions

The highly efficient Padé Via Lanczos method was shown to be a viable approach for computing statistical Stark broadening of spectral lines. Moreover, the method allows for efficient calculation of the average over the microfield distribution so that it can be carried out with confidence in the results. It is important to note that the PVL method is an iterative algorithm and makes no compromises on the physics of the problem. The numerical accuracy is

controlled using a straightforward scheme to determine convergence of the Lanczos iterations. The simple examples considered here served to illustrate the advantages of the PVL method over the traditional approach. It is expected that for large matrices and relatively smooth field-dependent line shape, the advantages can be even more dramatic.

The PVL method does have potential deficiencies. In particular, the Lanczos algorithm can experience numerical inaccuracies. The problem is related to loss of orthogonality in the Lanczos vectors. Here, due to the initial operational cost of forcing the field-dependent line shape function to a form suitable for the application of the PVL method, the straightforward Gram Schmidt orthogonalization procedure, often considered too expensive in other applications, should be robust with relatively small additional computational cost.

The main difficulty in a successful application of the PVL method is determining convergence of the Lanczos iterations. The procedure sketched here was based on direct evaluation of the quantity of interest, the integration over the quasi-static field. This is in principle a consistent approach that in practice needs further investigation.

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Appendix

The Lanczos method

A detailed and thorough presentation of the Lanczos process for complex, non-symmetric matrices is provided elsewhere [7,15]. Nevertheless, this Appendix contains practical information that is useful in the implementation of the Padé Via Lanczos (PVL) approach.

A.1 Description

The goal is an efficient method for evaluating

$$\ell^t (I - \varepsilon C)^{-1} r \quad (\text{A.1.1})$$

where C is a complex, non-symmetric matrix. The tridiagonalization of C is accomplished using the Lanczos Algorithm 7.42 of Ref. 15. The following description expands briefly on the explanation in [7,15], appropriately modified for complex non-symmetric matrices.

The Lanczos method for non-symmetric complex matrices can be considered as an iterative approach for generating a pair of bi-hermitian conjugate spaces. Given a complex non-symmetric matrix, C , and a pair of vectors, ℓ and r , one generates two Krylov spaces, which for k iterations are given by

$$\left\{ \ell, C^h \ell, (C^h)^2 \ell, \dots, (C^h)^{k-1} \ell \right\} \quad (\text{A.1.2})$$

and

$$\left\{ r, Cr, C^2 r, \dots, C^{k-1} r \right\} \quad (\text{A.1.3})$$

At each iteration, the Lanczos method generates Krylov spaces in succession by multiplying the matrix and its Hermitian conjugate with the current Lanczos vectors p_i and q_i where

$$p_i^h q_j = \delta_{ij} \quad (\text{A.1.4})$$

and the matrices with columns formed by the vectors p_i and q_i , which are denote by P and Q , respectively, satisfy the relations in Eqs. (2.1.5) and (2.1.6).

A simplification occurs when the starting vectors are chosen as

$$\begin{aligned} p_1 &= \ell / \sqrt{\bar{z}} \\ q_1 &= r / \sqrt{z} \end{aligned} \quad (\text{A.1.5})$$

where the bar denotes complex conjugate and the scaling factor

$$z = \ell^h r \quad (\text{A.1.6})$$

which are not affected by the Modified Gram Schmidt procedure (see Sect. 2.3) and satisfy Eq. (A.1.4). Then, it follows that

$$c^h Q = e_1^t \quad (\text{A.1.7})$$

$$P^h r = e_1 \quad (\text{A.1.8})$$

where $e_1 = [1, 0, \dots, 0]^t$ is the first unit vector of length k , the number of Lanczos iterations. Hence, Eq. (2.1.4) can be rewritten as

$$J_k(\omega; \varepsilon) = -\pi^{-1} \text{Im} \left\{ z e_1^t [I - (\varepsilon - \varepsilon_o) T_k]^{-1} e_1 \right\} \quad (\text{A.1.9})$$

This is an important result since only the [1,1] element of $[I - (\varepsilon - \varepsilon_o) T_k]^{-1}$ is required. It is stressed that the algorithm must be implemented with “rebiorthogonalization” described in the comment corresponding to Line 17 of Algorithm 7.42 in Ref. 15. Also note the correction to Line 11 of the same algorithm,

$$\beta_{j+1} = \sqrt{\omega_j} \quad (\text{A.1.10})$$

without absolute values. Here ω_j is a variable in the algorithm not to be confused with the frequency variable, ω , used in the line shape function.

A.2 Recursion relation

Since T_k is a tridiagonal matrix, it is possible to derive a Padé expansion for the [1,1] element in terms of ε . In practice, however, the evaluation of Eq. (A.1.9) can be done with a recursion relation. After performing k steps of the Lanczos algorithm, the resulting tridiagonal matrix is

$$T_k = \begin{bmatrix} \alpha_1 & \gamma_2 & & & \\ \beta_2 & \alpha_2 & \gamma_3 & & \\ & \beta_3 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \gamma_k \\ & & & \beta_k & \alpha_k \end{bmatrix} \quad (\text{A.2.1})$$

The following recursion formulas can be used to evaluate $f(\varepsilon)$. Define

$$d_k = 1 + \varepsilon \alpha_k \quad (\text{A.2.2})$$

and for $2 \leq n \leq k$

$$d_{n-1} = (1 + \varepsilon \alpha_{n-1}) - \varepsilon^2 \frac{\beta_n \gamma_n}{d_n} \quad (\text{A.2.3})$$

Then

$$J_k(\omega; \varepsilon) = \frac{z}{d_1} \quad (\text{A.2.4})$$

where z is the scaling factor in Eq. (A.1.6).

A.3 Numerical difficulties

The remarkable savings offered by the Lanczos method application to spectral line broadening should not blind one to the numerical problems that may arise during the calculations. Note that these difficulties are not insurmountable but do deserve careful attention. Some of the main issues are discussed below.

Although unlikely, the Lanczos method can fail even with full bi-orthogonalization. The specific ways in which this failure can occur are discussed in Ref. 15, and the appropriate stopping conditions are incorporated in Algorithm 7.42 in that reference. In case of failure, it may be necessary to use more sophisticated stabilization schemes such as the look-ahead Lanczos [8].

Since in the PVL method the evaluation of $J(\omega; \varepsilon)$ is efficient, the accuracy of the numerical integration over the quasi-static Stark field can be assured by using an adaptive quadrature without incurring a large penalty. An alternative approach is to optimize the field mesh. The latter requires the eigenvalues of a complex non-symmetric tridiagonal matrix and the usual efficient algorithm can be unstable [7]. It may be necessary to resort to the more expensive Schur decomposition of the tridiagonal system to obtain the eigenvalues.

The procedure to determine the number of Lanczos iterations needs to be robust. Since convergence with increasing numbers of iterations is erratic, it is not easy to determine when the process has converged. It may be necessary to use many more than the optimal number of iterations to ensure convergence. In connection with this problem is the range of integration over the field, which is not known in advance. It may be necessary to confirm that important features lying at large values of the microfield are not neglected.

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Figure captions

Fig. 1 $J_k(\omega;\varepsilon)$ versus field at $\hbar\omega = 3.02\text{ eV}$ using $\varepsilon_o = 0$ at $N_e = 10^{16}\text{ cm}^{-3}$ and $T = 1\text{ eV}$ for several values of k .

Fig. 2 Same as Fig. 2 using $\varepsilon_o = 2.4\varepsilon_H$.

Fig. 3 Average of $J(\omega;\varepsilon)$ over microfield distribution as a function of Lanczos iterations k relative to exact results using $\varepsilon_o = 0$ (*dash*) and $\varepsilon_o = 2.4\varepsilon_H$ (*solid*) at conditions of Fig. 1.

Fig. 4 Integrand in Eq. (1.1) versus field for various Lanczos iterations k at conditions of Fig. 1 with $\varepsilon_o = 0$.

Fig. 5 $J_k(\omega;\varepsilon)$ versus field at $\hbar\omega = 3.05\text{ eV}$ using $\varepsilon_o = 0$ at $N_e = 10^{16}\text{ cm}^{-3}$ and $T = 1\text{ eV}$ several values of k .

Fig. 6 Same as Fig. 5 using $\varepsilon_o = 7\varepsilon_H$.

Fig. 7 Average of $J(\omega;\varepsilon)$ over microfield distribution as a function of Lanczos iterations k relative to exact results using $\varepsilon_o = 0$ (*dash*) and $\varepsilon_o = 7\varepsilon_H$ (*solid*) at conditions of Fig. 5.

Fig. 8 Integrand in Eq. (1.1) versus field for various Lanczos iterations k at conditions of Fig. 5 with $\varepsilon_o = 0$.

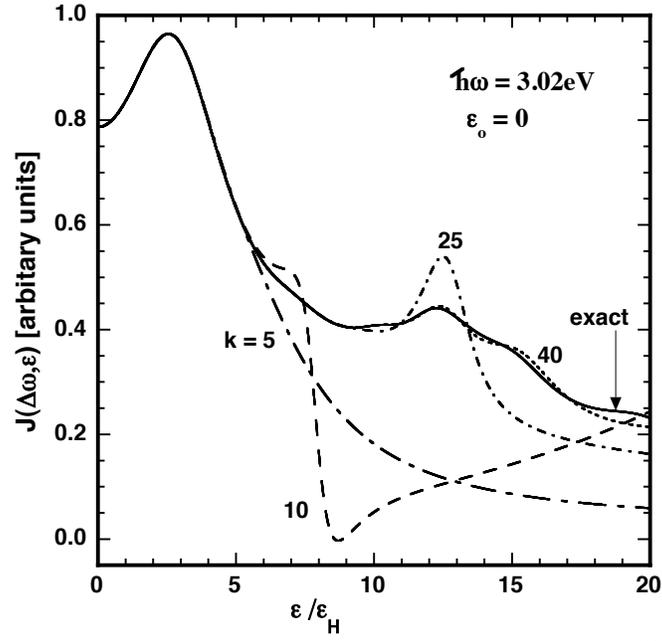


Fig. 1 $J_k(\omega; \epsilon)$ versus field at $\hbar\omega = 3.02 eV$ using $\epsilon_o = 0$ at $N_e = 10^{16} cm^{-3}$ and $T = 1 eV$ for several values of k .

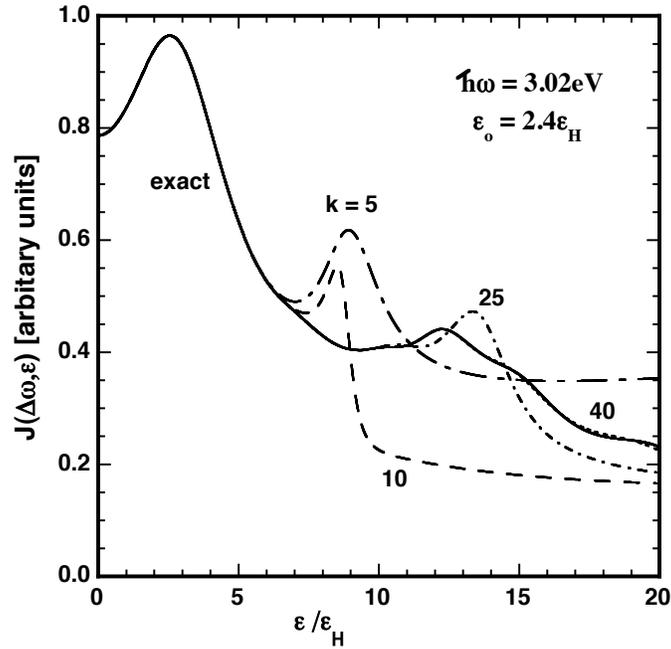


Fig. 2 Same as Fig. 2 using $\epsilon_o = 2.4\epsilon_H$.

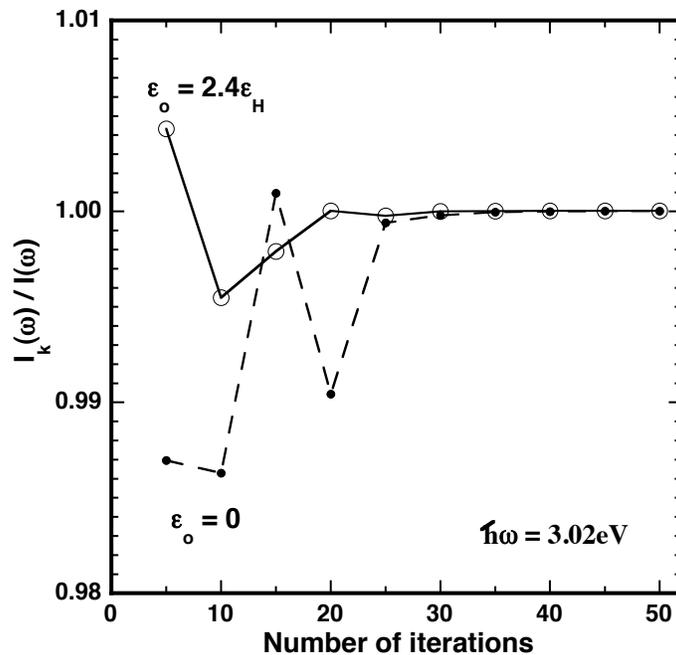


Fig. 3 Average of $J(\omega; \epsilon)$ over microfield distribution as a function of Lanczos iterations k relative to exact results using $\epsilon_o = 0$ (dash) and $\epsilon_o = 2.4\epsilon_H$ (solid) at conditions of Fig. 1.

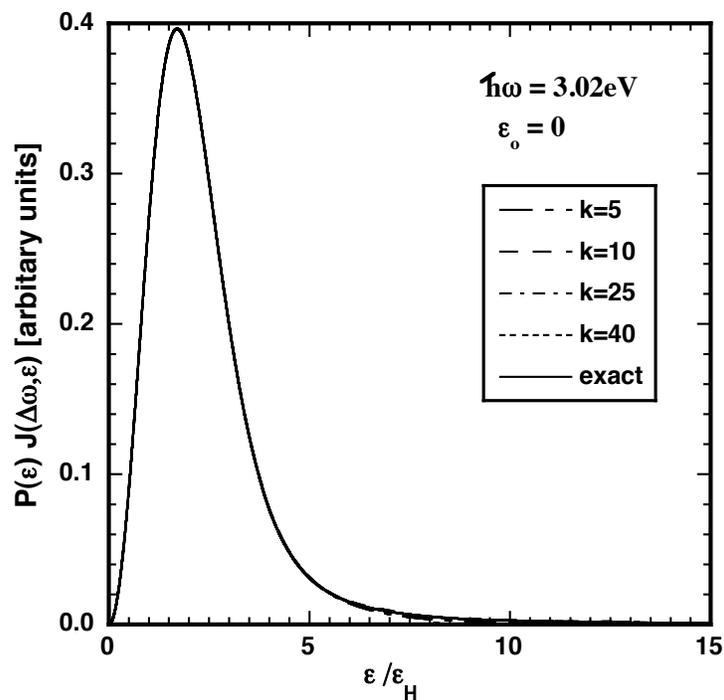


Fig. 4 Integrand in Eq. (1.1) versus field for various Lanczos iterations k at conditions of Fig. 1 with $\epsilon_o = 0$.

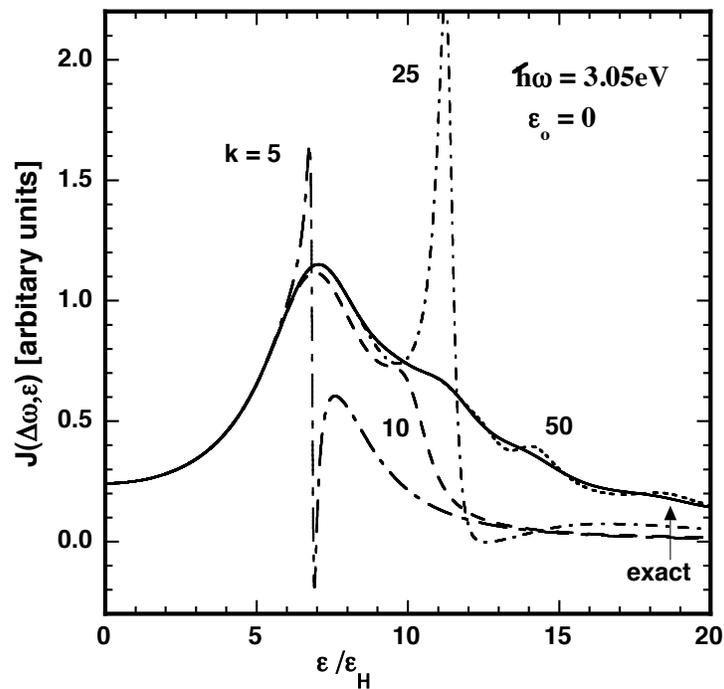


Fig. 5 $J_k(\omega; \epsilon)$ versus field at $\hbar\omega = 3.05 \text{ eV}$ using $\epsilon_o = 0$ at $N_e = 10^{16} \text{ cm}^{-3}$ and $T = 1 \text{ eV}$ several values of k .

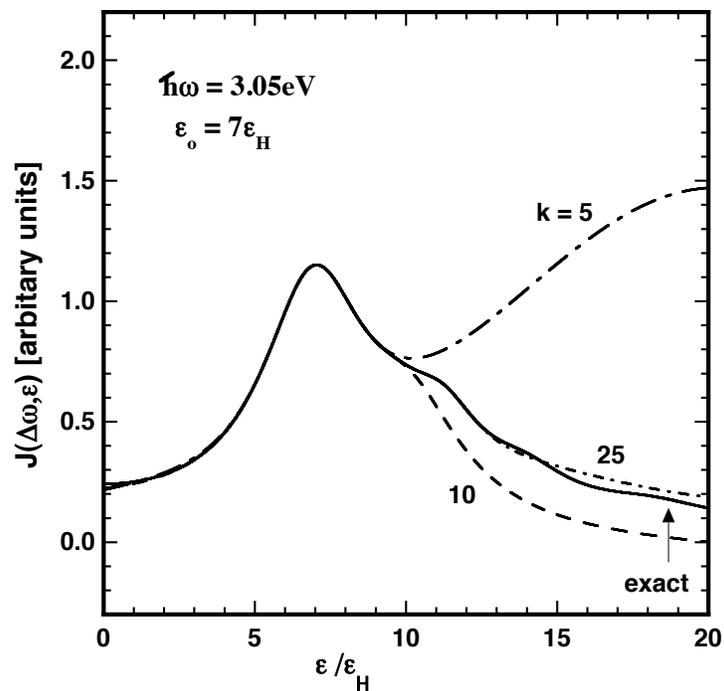


Fig. 6 Same as Fig. 5 using $\epsilon_o = 7\epsilon_H$.

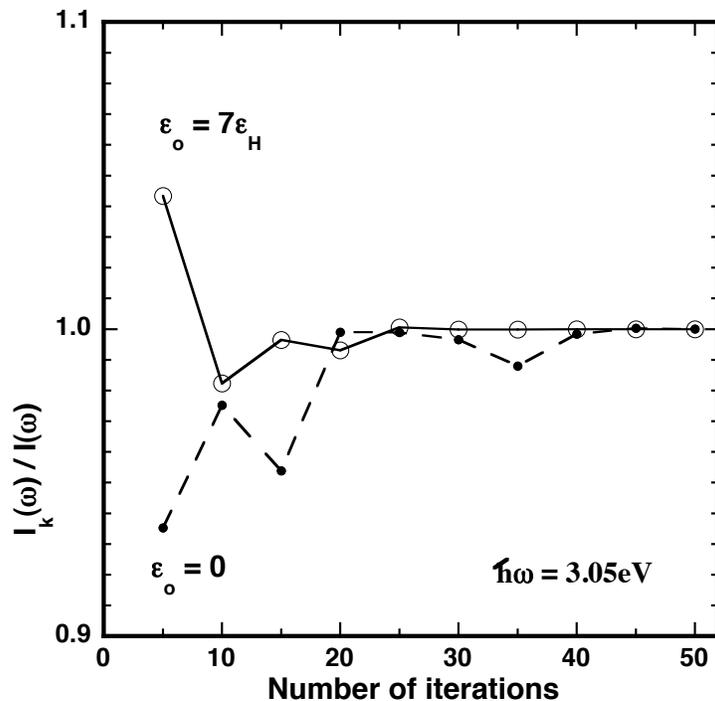


Fig. 7 Average of $J(\omega; \epsilon)$ over microfield distribution as a function of Lanczos iterations k relative to exact results using $\epsilon_o = 0$ (dash) and $\epsilon_o = 7\epsilon_H$ (solid) at conditions of Fig. 5.

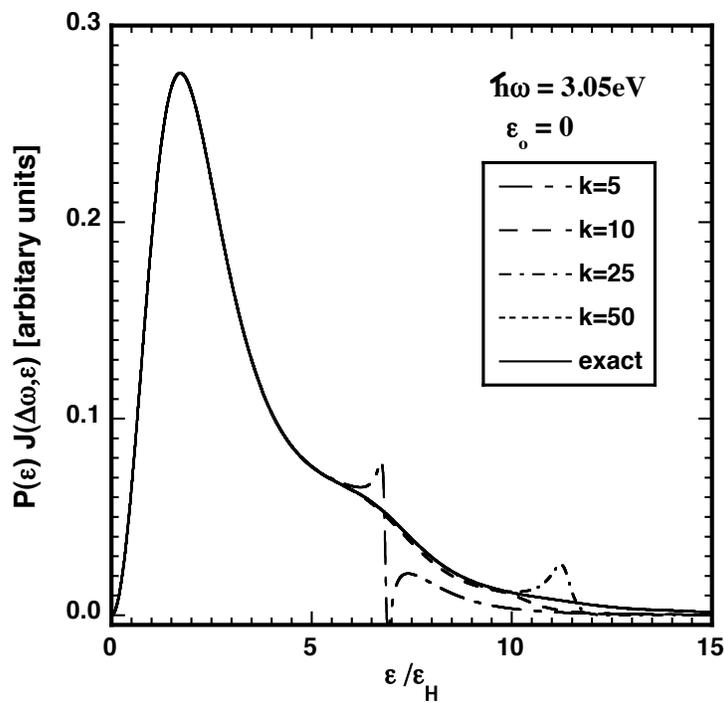


Fig. 8 Integrand in Eq. (1.1) versus field for various Lanczos iterations k at conditions of Fig. 5 with $\epsilon_o = 0$.